Supporting Information

Figure S1. The run sheet provided a method of reporting experimental details associated with hydrogen sorption measurements at a specific temperature.

National Renewable Energy Laboratory

INTER-LABORATORY COMPARISON RUN SHEET

INSTRUCTIONS				
Please fill out a run sheet for each measurement. You may want to fill out the fields that will be common for all measurements and then save this file so you do not have to fill in those fields every time.				
Please provide isotherm data calculated as excess gravimetric (wt%), excess volumetric (g H_2/L) and total volumetric (g H_2/L) in either tab-delimited format or an Excel spreadsheet. See the instruction sheet for additional details. If you correct for helium adsorption that occurs during the calibration, please supply both the corrected and uncorrected data if possible.				
If you have any questions call or email Katherine Hurst (303-384-7673; katherine.hurst@nrel.gov)				
LABORATORY INFORMATION				
Laboratory Institution		**Person filling out run sheet**		
Phone number for person		**E-mail for person**		
Filename(s) for this data:				
NOTE: The above information will be removed when the final results are reported. Laboratories will be identified anonymously using a randomly assigned number.				
SAMPLE TYPE:	☐ **Sample 1 or** ☐ **Sample 2**			
SAMPLE PREPARATION (skip if null measurement data)				
SAMPLE MASS				
Initial Mass:	±	mg	Date:	
After degas (optional):	±	mg	Date:	
Final Mass:	±	mg	Date:	
SAMPLE DEGAS	**Begin Date:**		**End Date:**	
Base Vacuum Pressure:	Units:			
Degas Protocol: ☐ **Degas protocol followed** ☐ **Degas protocol exception (explain)**				
Degas Explanation:				
Was sample exposed to air after degas and prior to measurement? ☐ **No** ☐ **Yes (explain)**				
Air Exposure Explanation:				
MEASUREMENT INFORMATION				
Measurement Method: ☐ **Gravimetric** ☐ **Volumetric** ☐ **Other:**			☐ **Static** ☐ **Dynamic**	
Measurement Temperature: ☐ **Liquid Nitrogen** ☐ **Ambient:** **K**			**If dynamic, flow rate:**	
Hydrogen Purity: **%**	**Additional purifier used?** ☐**Yes** ☐**No**			
Base Vacuum Pressure:	Units:			
Sequence order: ☐ **He calibration done first**			☐ **H_2 measurement done first**	
Equilibrium time/step: (min.)	**Total time for measurement:** min.			
Temperature stability: **Standard Deviation:** **K**	**Pressure Sensor Accuracy:** **%** ☐ **FS** ☐**Reading**			
Equation of State: ☐ **Ideal** ☐**Real:** **Model:**				
CALIBRATION				
Helium adsorption correction:	**Supplied data has** **Method:** no correction **if other, explain:**			
Skeletal Density:	☐ **Not Measured** ☐ **Measured:**	**g/cm^3**	**Method used:**	
Packing Density:	**Measured:**	**g/cm^3**	**Method used:**	
COMMENTS				

Outlier Analysis for Skeletal and Packing Densities

With regard to the measured values of the skeletal and packing densities, there were some values that were significantly different than the majority of the values. It therefore raises the question if these particular values should be considered as outliers and not included in the main analysis of densities. To address this question, we applied accepted outlier statistical tests to these data using the generalized extreme Studentized deviate (ESD) protocol.[20-21] The ESD test is similar to the Grubbs test[22] for a single outlier, but allows for multiple outliers. With the ESD test, the maximum number of outliers, *r*, is specified, and the test is repeated starting from a single outlier up to the maximum number. For each test, the test statistic R_i is computed:

$$R_i = \frac{max_i|x_i - \bar{x}|}{s} \qquad (1)$$

Where R_i is the absolute value of the maximum deviation of the data samples obtained for point x_i from the mean, $\bar{x}$, divided by the standard deviation of the sample, *s*. Subsequent tests are performed with the previous maximum deviation datum point removed and the mean and standard deviation recomputed with the previous maximum datum point removed. The test statistics are compared with the corresponding critical values, λ_i, derived from a relation associated with the t-distribution.[21]

$$\lambda_i = \frac{(n-i)\, t_{p,\ n-i-1}}{\sqrt{(n-i-1+t^2_{p,\ n-i-1})(n-i-1)}} \qquad i = 1, 2, \ldots, r \qquad (2)$$

Where n is the number of data points in the set, $t_{p,\nu}$ is the 100p percentage point from the t distribution with ν degrees of freedom and

$$p = 1 - \frac{\alpha}{2(n-i+1)} \quad (3)$$

with α the significance level. This test was applied to the data for each density for each sample type looking for a maximum of 5 outliers at a significance level of 0.5%, i.e., there should only be a 0.5% chance that we are eliminating valid data point(s). The tests identified 1 outlier each in the packing density for Sample 1 and 2, and in the skeletal density for Sample 1, and it identified 3 outliers for the skeletal densities for Sample 2.

Interpolated Values of Adsorption Isotherms

In order to be able to compare the pressure-composition-temperature (PCT) data statistically, it is necessary to do so at a set of common pressures for all the isotherms. This was accomplished by choosing a set of common pressures and then interpolating the different isotherm data sets to those pressures. A linear interpolation algorithm between each pair of actual data points was chosen to provide those values as it was straightforward to implement and guaranteed that all the actual data points would be captured. No extrapolation was performed outside the minimum or maximum of the actual pressures that were measured. For this analysis, only adsorption data was considered. A list of all the interpolated points is given in Tables S1 - S12. The results are then shown using box and whisker plots to assess the reproducibility. Note that the values listed in these tables show 3 significant digits in order to display in table format. All statistics (shown in Figures S2-S7, and the relative standard deviation shown in Fig 11) are calculated based on the interpolated data without limiting the number of significant digits.

Table S1. Interpolated Gravimetric Excess Capacities at Ambient Temperature – Sample 1
The numbers shown in the table are x10^{-3}, (the values should be multiplied by 10^{-3})

	Data Set Number and Capacity (wt%)														
Pressure (bar)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	7.81	7.95		10.1						7.95	7.55	8.01			23.0
2	15.4	15.8		20.3	15.4	12.6				15.6	15.1	15.9	30.3		32.0
4	30.6	31.5		40.3	33.4	26.3			19.0	30.7	30.0	31.2	45.7	33.7	48.0
8	60.2	62.8	64.2	67.8	67.3	53.7			43.0	59.2	58.4	60.5	76.5	61.5	76.0
10	74.1	77.3	78.7	81.1	82.4	675			55.1	72.7	72.1	74.0	91.5	75.4	90.0
12	88.0	91.8	93.3	93.9	97.8	81.0			67.2	85.7	85.9	87.5	107	88.6	103
15	108	113	114	113	121	98.5		104	85.3	105	105	107	129	108	123
17	120	128	127	126	137	110		115	97.5	117	118	119	144	121	137
20	139	150	145	144	158	128		133	116	135	136	137	164	139	
25	168	182	175	169	191	156		162	148		165	166	197	169	
30	195	213	202	194	221	185	180	189	168		192	193	224	195	
35	222	243	229	219	251	212	206	213	191		218	218	245	215	
40	246	272	255	244	280	236	231	239	220		242	240	267	231	
45	269	297	277	269	306	260	255	261	249		264	262	292	251	
50	291	323	299	291	331	282	276	283	279		285	282			
60	331	370	340	332	375	323	317	324	316		325	319		318	
70	367	417	375	371	419	360	354	362			361	352		363	
80	400	460	407	407	460	391	388	397				382		404	

90	428	493	435	442	419	421	429			408		444	
100			462		446	449	460			435		480	

Table S2. Interpolated Gravimetric Excess Capacities at Ambient Temperature – Sample 2
The numbers shown in the table are x 10^{-3}, (the values should be multiplied by 10^{-3}).

	Data Set Number and Capacity (wt%)													
Pressure (bar)	1	2	3	4	5	6	8	9	10	11	12	13	14	15
1	11.6	12.9		15.0		8.37			11.6	11.1	11.7		6.30	10.0
2	23.0	27.6		30.0	12.1	18.6		22.5	23.0	22.2	22.9	41.9	17.2	22.0
4	45.3	56.1		52.3	36.5	39.1	45.5	45.4	45.2	44.0	45.2	68.1	38.8	46.0
6	67.4	82.0	75.8	74.4	62.3	59.6	65.0	67.6	66.7	65.6	67.0	94.2	60.4	70.0
8	89.0	108	98.4	96.2	87.0	80.1	84.4	88.9	87.6	86.3	87.8	120	82.1	92.0
10	110	131	121	115	112	101	104	108	108	107	108	148	104	114
12	130	156	144	134	134	121	123	128	127	127	128	175	125	136
15	159	192	177	163	164	149	152	158	156	155	157	216	154	167
17	178	211	197	182	185	168	169	178	174	175	175	243	172	188
20	206	239	228	207	222	193	194	203	200	202	202	268	198	
25	251	298	277	248	282	238	237	245	242	246	0245	307	243	
30	294	357	320	289	326	276	277	285		285	285	346	283	
35	337	406	364	327	370	313	316	322		323	321	384	322	
40	375	455	405	361	412	350	352	355		356	356	421	359	
45	410	504	440	394	451	382	388	386		395	388	456	392	
50	442	554	476	424	490	415	421	416		427	419		426	
60	501	653	542	479	566	473	484	478		486	474		485	
70	552	725	602	533	622	5269	540			539	524		540	
80	597	813	657	582	677	575	595				564		591	
90	638	906	705	628		619	645				604		637	
100			750			659	691				641		677	

Table S3. Interpolated Gravimetric Excess Capacities at liquid N_2 temperature – Sample 1

	Data Set Number and Capacity (wt%)								
Pressure (bar)	2	3	4	5	8	9	10	14	15

1	1.73	1.77	1.45	1.63	1.40	1.68	1.76	1.53	1.69
2	2.01	2.07	1.93	2.03	1.67	1.94	2.07	1.69	1.99
4	2.57	2.38	2.31	2.36	2.21	2.37	2.36	2.00	2.28
6	2.68	2.54	2.50	2.55	2.71	2.50	2.52	2.32	2.44
8	2.78	2.66	2.63	2.72	2.78	2.63	2.62	2.64	2.54
10	2.88	2.73	2.70	2.79	2.86	2.71	2.70	2.69	2.62
12	2.98	2.79	2.76	2.86	2.93	2.78	2.76	2.73	2.67
15	3.13	2.85	2.85	2.93	3.04	2.87	2.83	2.80	2.73
17	3.21	2.88	2.87	2.98	3.07	2.92	2.86	2.84	2.77
20	3.25	2.91	2.90	3.02	3.10	3.00	2.90	2.88	2.80
25	3.30	2.94	2.96	3.07	3.16	3.11		2.90	
30	3.31	2.95	2.98	3.10	3.16	3.22		2.92	
35	3.29	2.93	2.97	3.10	3.16	3.31		2.91	
40	3.27	2.91	2.96	3.09	3.14	3.39		2.89	
45	3.23	2.88	2.95	3.08	3.11	3.46		2.86	
50	3.18	2.84	2.91	3.04	3.08	3.49		2.83	
60	3.06	2.75	2.84	2.97	2.99			2.75	
70	2.93	2.65	2.76	2.91	2.88			2.65	
80	2.79	2.54	2.67	2.83					
90	2.66	2.43							
100		2.33							

Table S4 Interpolated Gravimetric Excess Capacities at liquid N_2 temperature – Sample 2

	Data Set Number and Capacity (wt%)								
Pressure (bar)	2	3		5	8	9	10	14	15
1	2.58	2.74	2.18	2.53	2.17	2.35	2.72	2.35	2.71
2	3.10	3.32	3.15	3.12	2.81	2.87	3.24	2.83	3.23
4	3.71	3.83	3.55	3.69	3.81	3.64	3.71	3.78	3.71
6	4.03	4.06	3.79	3.97	3.96	3.88	3.96	4.03	3.97
8	4.14	4.26	4.04	4.24	4.12	4.11	4.12	4.18	4.14
10	4.25	4.37	4.28	4.34	4.27	4.24	4.24	4.33	4.26
12	4.36	4.49	4.40	4.44	4.43	4.37	4.33	4.48	4.36

15	4.53	4.58	4.49	4.57	4.53	4.48	4.43	4.55	4.46
17	4.61	4.64	4.54	4.62	4.57	4.55	4.48	4.60	4.50
20	4.63	4.69	4.63	4.70	4.62	4.65	4.54	4.66	
25	4.62	4.74	4.71	4.77	4.68	4.77	4.60	4.71	
30	4.58	4.76	4.72	4.81	4.68	4.90		4.72	
35	4.50	4.75	4.72	4.82	4.67	5.03		4.71	
40	4.40	4.73	4.71	4.80	4.63	5.10		4.68	
45	4.29	4.69	4.65	4.78	4.59	5.18		4.63	
50	4.16	4.64	4.60	4.74	4.53	5.22		4.58	
60	3.91	4.51	4.47	4.64	4.39			4.44	
70	3.65	4.38	4.33	4.51	4.24			4.30	
80	3.37	4.22	4.20	4.43				4.14	
90	3.11	4.07						3.97	
100		3.92							

Table S5 Interpolated Volumetric Excess Capacities at Ambient Temperature – Sample 1
The numbers shown in the table are x 10^{-2}, (the values should be multiplied by 10^{-2}).

	Data Set Number & Capacity (g-H_2 L^{-1})												
Pressure (bar)	1	2	3	4	5	6	7	8	9	10	11	12	14
1	2.75	2.49		3.71						2.91	3.10	2.88	
2	5.44	4.96		7.42	5.58	4.13				5.71	6.19	5.71	
4	10.8	9.89		14.8	12.1	8.61			6.98	11.2	12.3	11.2	11.9
6	16.1	14.8		20.0	18.9	13.1			11.2	16.5	18.2	16.6	16.9
8	21.2	19.7	24.4	25.1	24.4	17.6			15.6	21.6	23.9	21.7	21.8
10	26.1	24.3	29.9	30.1	29.8	22.1			20.0	26.6	29.5	26.6	26.7
12	30.9	28.8	35.5	34.8	35.4	26.6			24.4	31.4	35.2	31.5	31.4
15	37.9	35.7	43.5	41.9	44.0	32.3		36.4	30.8	38.3	43.0	38.5	38.3
17	42.3	40.3	48.2	46.6	49.7	36.1		40.5	35.2	42.8	48.2	42.9	42.9
20	49.0	47.1	55.3	53.3	57.1	41.8		46.6	42.0	49.2	55.8	49.5	49.6
25	59.4	57.1	66.7	62.6	69.1	51.3		56.9	53.4		67.6	59.8	59.9
30	68.9	67.0	77.0	71.9	80.2	60.7	60.2	66.4	60.9		78.8	69.3	69.3
35	78.1	76.2	87.4	81.2	91.2	69.6	68.7	75.0	69.2		89.2	78.3	76.4
40	86.7	85.4	97.2	90.5	101	77.6	77.2	83.7	79.4		99.2	86.3	82.2

45	94.8	93.4	106	99.9	111	85.5	85.1	91.7	90.0	108	94.3	88.9
50	103	101	114	108	120	92.7	92.2	99.3	101	117	101	
60	117	116	130	123	136	106	106	114	114	133	114	113
70	129	131	143	138	152	118	118	127		148	127	129
80	141	145	155	151	167	129	130	139			138	144
90	151	155	166	164		138	141	151			147	158
100			176			147	150	161			157	171

Table S6 Interpolated Volumetric Excess Capacities at Ambient Temperature – Sample 2
The numbers shown in the table are x 10^{-2}, (the values should be multiplied by 10^{-2}).

	Data Set Number & Capacity (g-H_2 L^{-1})											
Pressure (bar)	1	2	3	4	5	6	8	9	10	11	12	14
1	2.22	2.67		3.50		2.05			4.40	1.74	2.45	1.73
2	4.39	5.71		7.00	4.99	4.55		4.98	8.70	3.48	4.81	4.69
4	8.64	11.6		12.1	15.0	9.56	11.3	10.0	17.1	6.90	9.48	10.6
6	12.9	17.0	22.0	17.3	25.7	14.6	16.2	14.9	25.3	10.3	14.1	16.5
8	17.0	22.3	28.6	22.2	35.9	19.6	21.2	19.5	33.2	13.6	18.4	22.4
10	21.0	27.2	35.1	26.6	46.1	24.6	26.1	23.9	40.8	16.7	22.6	28.3
12	24.8	32.2	41.7	31.0	55.2	29.6	31.0	28.3	48.3	19.9	26.8	34.3
15	30.5	39.7	51.3	37.6	67.9	36.4	38.1	34.8	59.0	24.4	32.9	42.0
17	34.1	43.6	57.3	42.0	76.3	40.8	42.5	39.2	65.9	27.4	36.7	47.0
20	39.5	49.5	66.3	47.8	92.0	47.3	49.0	44.9	76.0	31.7	42.4	54.3
25	48.1	61.7	80.5	57.3	116	58.1	59.8	54.2	91.7	38.5	51.5	66.6
30	56.3	73.8	93.2	66.7	135	67.6	69.8	62.9		44.8	59.8	77.4
35	64.6	84.1	106	75.6	153	76.7	79.8	71.0		50.9	67.6	88.1
40	71.9	94.3	118	83.3	171	85.6	89.0	78.3		56.6	74.9	98.4
45	78.6	105	128	91.0	187	93.6	98.0	85.2		62.0	81.7	108
50	84.9	115	139	97.9	203	102	106	92.0		67.2	88.1	117
60	96.2	135	158	111	234	116	122	106		76.5	99.9	133
70	106	150	176	123	258	129	136			85.0	110	148
80	115	168	192	135	281	141	150				119	162
90	123	187	205	145		152	163				127	175
100			219			162	175				135	186

Table S7. Interpolated Volumetric Excess Capacities at liquid N_2 temperature – Sample 1

	Data Set # & Capacity (g-H_2 L^{-1})							
Pressure (bar)	2	3	4	5	8	9	10	14
1	5.44	6.86	5.47	5.98	4.98	6.17	6.56	5.50
2	6.32	8.02	7.27	7.49	5.96	7.14	7.73	6.08
4	8.07	9.25	8.76	8.77	7.93	8.78	8.83	7.25

6	8.43	9.91	9.47	9.47	9.75	9.27	9.43	8.43
8	8.74	10.3	10.0	10.1	10.0	9.77	9.84	9.60
10	9.05	10.7	10.3	10.4	10.3	10.1	10.1	9.78
12	9.36	10.9	10.5	10.7	10.6	10.3	10.4	9.94
15	9.83	11.2	10.8	11.0	11.0	10.7	10.6	10.2
17	10.1	11.3	10.9	11.1	11.1	10.9	10.8	10.4
20	10.2	11.4	11.2	11.3	11.2	11.2	10.9	10.5
25	10.3	11.5	11.3	11.5	11.4	11.6		10.6
30	10.4	11.5	11.4	11.6	11.4	12.0		10.6
35	10.3	11.5	11.4	11.7	11.4	12.4		10.6
40	10.3	11.4	11.3	11.5	11.3	12.7		10.5
45	10.1	11.3	11.2	11.5	11.2	12.9		10.4
50	9.97	11.1	11.1	11.4	11.1	13.0		10.3
60	9.62	10.8	10.8	11.1	10.8			10.0
70	9.20	10.4	10.5	10.8	10.4			9.63
80	8.76	9.92	10.1	10.5				
90	8.35	9.48						
100		9.05						

Table S8. Interpolated Volumetric Excess Capacities at liquid N_2 temperature – Sample 2

	Data Set # & Capacity (g-H_2 L^{-1})							
Pressure (bar)	2	3	4	5	8	9	10	14
1	5.33	8.16	5.16	10.7	5.70	5.30	10.6	6.57
2	6.43	9.96	7.49	13.3	7.41	6.51	12.7	7.96
4	7.69	11.6	8.47	15.8	10.1	8.31	14.6	10.7
6	8.35	12.3	9.08	17.1	10.5	8.88	15.6	11.5
8	8.58	12.9	9.69	18.3	11.0	9.43	16.3	11.9
10	8.81	13.3	10.2	18.7	11.4	9.75	16.8	12.3
12	9.03	13.6	10.6	19.1	11.8	10.0	17.1	12.8
15	9.37	13.9	10.8	19.7	12.1	10.3	17.5	13.0
17	9.54	14.1	10.9	20.0	12.2	10.5	17.8	13.2
20	9.58	14.3	11.2	20.3	12.4	10.7	18.0	13.3
25	9.57	14.4	11.4	20.6	12.5	11.0	18.3	13.5

30	9.48	14.5	11.4	20.8	12.5	11.3		13.5
35	9.36	14.5	11.4	20.9	12.5	11.6		13.5
40	9.11	14.4	11.4	20.8	12.4	11.8		13.4
45	8.89	14.3	11.2	20.7	12.3	12.0		13.3
50	8.62	14.1	11.1	20.5	12.1	12.1		13.1
60	8.08	13.7	10.8	20.0	11.7			12.7
70	7.55	13.3	10.4	19.5	11.3			12.2
80	6.97	12.8	10.1	19.1				11.8
90	6.43	12.3						11.3
100		11.8						

Table S9. Interpolated Total Volumetric Capacities at Ambient Temperature – Sample 1
Values shown in table are displayed as x 10^{-2}, (The value is determined by multiplying by 10^{-2}).

	Data Set # & Capacity (g-H_2 L^{-1})												
Pressure (bar)	1	2	3	4	5	6	7	8	9	10	11	12	14
1	9.63	9.42		10.6						9.72	9.85	9.66	
2	19.2	18.8		21.1	19.0	17.8				19.3	19.7	19.3	
4	38.2	37.6		42.2	38.9	36.0			31.2	38.4	39.3	38.3	38.9
6	57.2	56.2		61.0	59.1	54.2			47.5	57.2	58.7	57.2	57.2
8	76.0	74.9	79.3	79.8	77.9	72.4			63.9	75.9	77.8	75.8	75.5
10	94.5	93.1	98.5	98.4	96.6	90.5			80.3	94.4	96.9	94.1	93.8
12	113	111	118	117	116	109			96.8	113	116	112	112
15	140	139	146	144	144	135		137	121	140	144	140	138
17	158	157	164	162	163	152		154	137	158	163	157	156
20	185	184	192	189	190	178		180	163	184	190	184	183
25	229	227	237	231	235	221		224	203		234	227	226
30	272	271	280	274	278	264	296	266	240		278	270	268
35	314	314	324	316	322	306	343	307	277		321	311	307
40	356	356	367	359	364	347	390	348	316		364	352	345
45	397	397	408	401	406	387	436	389	356		406	392	384
50	437	437	449	441	447	427	481	428	395		446	432	
60	515	518	529	521	526	505	570	506	466		526	509	503

70	592	596	607	599	604	581	657	583		603	584	581
80	667	674	682	675	680	654	741	657			657	658
90	739	747	755	751		725	825	730			728	733
100			827			796	906	801			799	806

Table S10. Interpolated Total Volumetric Capacities at Ambient Temperature – Sample 2
Values shown in table are displayed as x 10^{-2}, (The value is determined by multiplying by 10^{-2}).

	Data Set # & Capacity (g-H_2 L^{-1})											
Pressure (bar)	1	2	3	4	5	6	8	9	10	11	12	14
1	9.73	8.74		10.8		9.13			11.7	9.10	10.1	8.64
2	19.4	18.2		21.7	18.0	18.7		18.9	22.8	18.2	20.1	18.5
4	38.6	37.2		41.4	41.1	37.9	39.8	37.9	44.6	36.5	40.1	38.2
6	57.7	56.4	64.6	61.1	64.7	57.1	58.8	56.6	66.2	54.6	59.9	57.9
8	76.8	75.5	85.2	80.7	87.8	76.2	77.8	75.2	87.6	72.5	79.4	77.7
10	95.6	93.6	106	99.6	111	95.4	96.9	93.3	109	90.4	98.7	97.4
12	114	112	126	118	133	115	116	112	127	108	118	117
15	142	139	157	147	165	142	144	139	161	134	147	145
17	160	156	177	166	186	161	162	157	181	152	165	164
20	188	182	207	193	221	188	190	183	211	179	193	192
25	233	226	256	238	277	234	235	226	261	221	239	238
30	278	271	303	283	327	278	280	269		263	284	282
35	322	313	350	328	377	321	324	311		305	328	326
40	365	355	396	370	426	364	368	351		346	372	370
45	408	397	440	413	473	406	411	391		387	414	412
50	449	439	484	454	520	448	453	431		427	456	454
60	531	522	570	536	613	529	535	510		506	538	536
70	610	599	654	617	697	608	616			583	618	615
80	688	679	735	696	779	686	695				695	693
90	763	758	813	773		761	772				770	769
100			890			835	847				845	842

Table S11. Interpolated Total Volumetric Capacities at liquid N_2 temperature – Sample 1

	Data Set # & Capacity (g-H_2 L^{-1})							
Pressure (bar)	2	3	4	5	8	9	10	14
1	5.71	7.12	5.74	6.25	5.29	6.41	6.83	5.81
2	6.85	8.54	7.81	8.00	6.59	7.61	8.26	6.71
4	9.14	10.3	9.83	9.82	9.17	9.73	9.88	8.51
6	10.1	11.5	11.1	11.1	11.6	10.7	11.0	10.3
8	10.9	12.5	12.2	12.2	12.5	11.7	12.0	12.1
10	11.8	13.3	13.0	13.0	13.4	12.5	12.8	12.9
12	12.6	14.1	13.8	13.8	14.4	13.2	13.6	13.7
15	13.9	15.1	14.9	15.0	15.7	14.3	14.6	15.0
17	14.7	15.8	15.6	15.7	16.5	15.0	15.3	15.8
20	15.7	16.7	16.5	16.6	17.6	16.0	16.3	16.9
25	17.3	18.2	18.2	18.2	19.4	17.7		18.6
30	18.7	19.6	19.7	19.7	21.1	19.3		20.3
35	20.1	20.9	21.0	21.1	22.8	21.0		21.9
40	21.4	22.2	22.4	22.4	24.4	22.5		23.5
45	22.7	23.4	23.8	23.8	25.9	24.0		25.1
50	23.9	24.6	25.8	25.0	27.4	25.3		26.6
60	26.3	26.9	27.5	27.4	30.3			29.5
70	28.6	29.0	29.8	29.8	33.0			32.2
80	30.7	31.0	32.0	31.9				
90	32.6	32.9						
100		34.6						

Table S12. Interpolated Total Volumetric Capacities at liquid N_2 temperature – Sample 2

	Relative Absolute Standard Deviation (%)							
Pressure (bar)	2	3	4	5	8	9	10	14
1	5.59	8.43	5.45	11.0	6.01	5.57	10.8	6.87
2	6.94	10.5	8.07	13.8	8.04	7.05	13.2	8.53
4	8.72	12.6	9.62	16.8	11.4	9.40	15.6	11.9

6	9.92	13.9	10.8	18.6	12.4	10.5	17.2	13.2
8	10.7	15.1	12.0	20.3	13.5	11.6	18.4	14.2
10	11.4	16.0	13.2	21.3	14.6	12.5	19.4	15.2
12	12.2	16.9	14.1	22.2	15.7	13.4	20.3	16.2
15	13.3	18.0	15.2	23.6	16.9	14.5	21.6	17.3
17	14.0	18.8	15.9	24.4	17.7	15.2	22.3	18.1
20	14.9	19.8	17.0	25.5	18.8	16.3	23.4	19.1
25	16.2	21.3	18.7	27.2	20.6	18.0	25.0	20.7
30	17.5	22.8	20.3	28.7	22.3	19.8		22.3
35	18.7	24.2	21.8	30.1	24.0	21.5		23.7
40	19.9	25.5	23.3	31.4	25.5	23.1		25.2
45	21.0	26.8	24.6	32.6	27.1	24.8		26.5
50	22.1	28.0	26.0	33.8	28.6	26.3		27.8
60	24.2	30.4	28.6	35.9	31.4			30.3
70	26.2	32.6	31.1	37.8	34.1			32.6
80	28.0	34.6	33.4	39.9				34.8
90	29.8	36.5						36.8
100		38.2						

Table S13. Statistical Analysis for the Gravimetric Excess Capacities of different data sets at ambient temperature evaluated at various pressures – Sample 2. This data is plotted in Figure S2A.

		Relative Absolute Standard Deviation (%)			
Data Set	Sample Mass (mg)	2 bar	10 bar	25 bar	60 bar
7	2.01	4.81	1.13	1.30	1.94
2	0.310	25.8	18.6	17.2	27.7
3	1.08		9.09	8.85	6.14
4	1.03	36.7	3.90	2.41	6.31
5	0.475	44.8	0.667	10.8	10.7
6	0.936	15.0	9.29	6.58	7.37
8	0.204		6.39	6.76	5.40
9	0.384	2.69	2.25	3.50	6.40
10	0.2335	4.90	2.80	4.91	

11	0.890	1.40	3.89	3.33	4.90
12	1.42	4.70	2.80	3.65	7.20
14	0.782	21.7	6.54	4.35	5.04
15	0.183	0.516	2.81		

Table S14. Statistical Analysis for the Gravimetric Excess Capacities of different data sets at liquid N_2 temperature evaluated at various pressures – Sample 2. This data is plotted in Figure S2B.

		Relative Absolute Standard Deviation (5%)			
Data Set	Sample Mass (mg)	2 bar	10 bar	25 bar	60 bar
2	0.310	7.95		10.1	
3	1.08	15.8		20.3	15.4
4	1.03	31.5		40.3	33.4
5	0.475	62.8	64.2	67.8	67.3
8	0.204	77.3	78.7	81.1	82.4
9	0.384	91.8	93.3	93.9	97.8
10	0.234	113	114	113	121
14	0.782	128	127	126	137
15	0.183	150	145	144	158

Statistical Analysis of Interpolated Data

Within the box, the solid line indicates the median, and the dot indicates the mean value amongst all participants at this pressure. The upper and lower limits of the box represent the 75% quartile and 25% quartile of the data respectively. The whiskers show the boundary of 10% (lower whisker) and 90% (upper whisker) of the reported data. The graph at the top of these figures show the number of data points analyzed at each pressure. Not all laboratories have the capability to measure adsorption to the same pressures and this accounts for the variation in the number of these points. These metrics provide a statistically relevant picture of the degree of data variation. The decrease in the variability at 100 bar is a result of the reduced number of data sets in the analysis.

Figure S2 Statistical analysis of excess gravimetric capacities at ambient temperatures for a) Sample 1, and b) Sample 2.

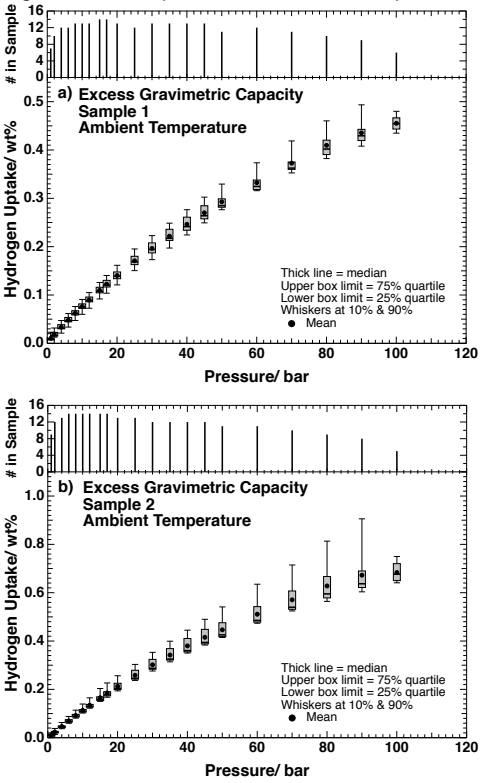

Figure S3 Statistical analysis of gravimetric excess capacities at liquid N_2 temperature for a) Sample 1, and b) Sample 2.

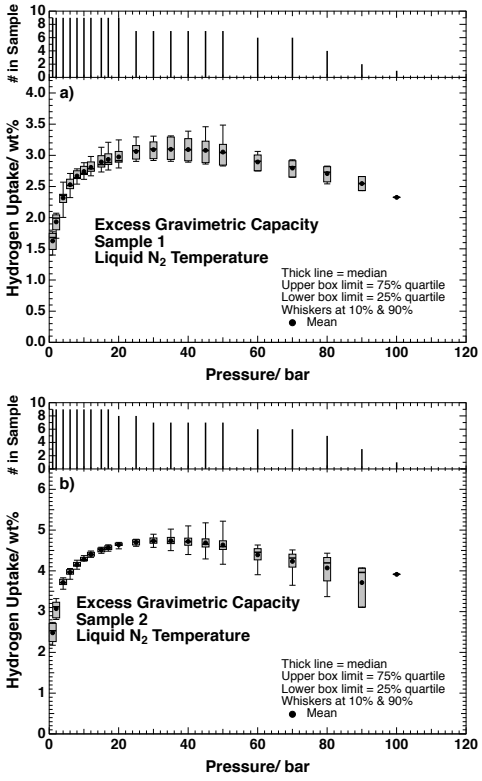

Figure S4 Statistical analysis of excess volumetric capacities at ambient temperature for a) Sample 1, and b) Sample 2.

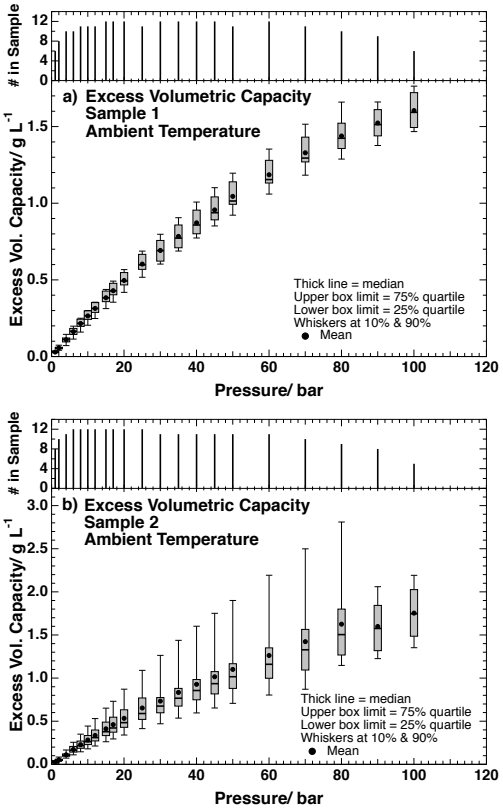

Figure S5 Statistical analysis of excess volumetric capacities at liquid N_2 temperatures for a) Sample 1, and b) Sample 2.

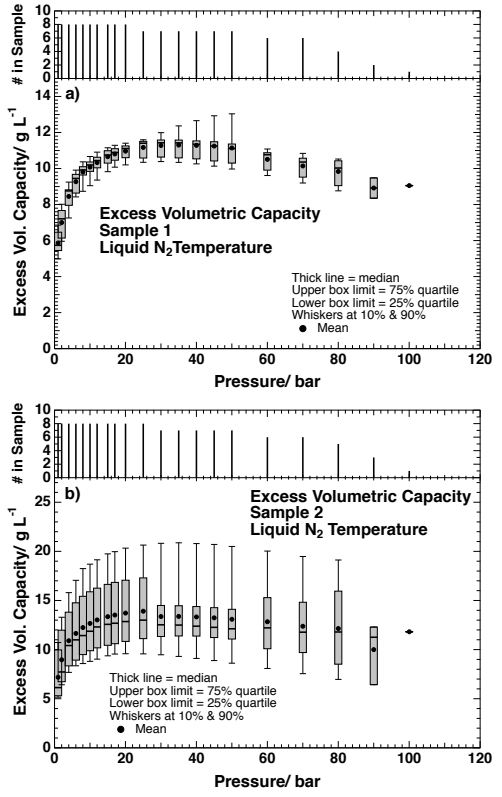

Figure S6 Statistical analysis of total volumetric capacities at ambient temperatures for a) Sample 1, and b) Sample 2.

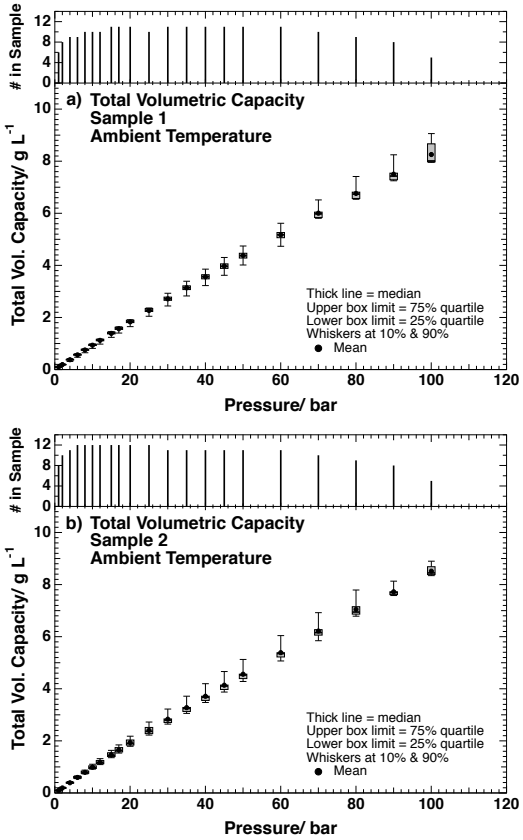

Figure S7 Statistical analysis of total volumetric capacities for a) Sample 1, and b) Sample 2.

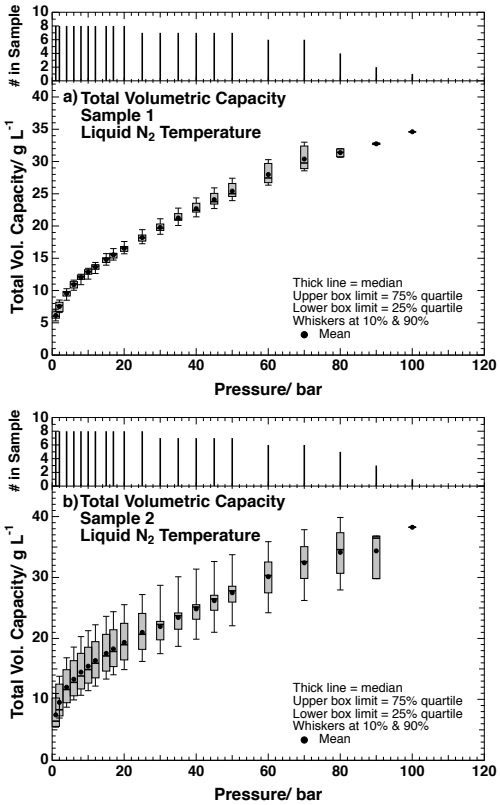

Figure S8. The relative absolute standard deviation of the excess gravimetric H_2 capacity as a function of sample mass for various pressures at a). ambient temperature and b). liquid N_2 temperature.